U.S.-JAPAN SEMINAR ON EVALUATION, COMPILATION, AND PRESENTATION OF PHYSICAL PROPERTY DATA AND DATA CENTER ACTIVITIES

Tokyo, Japan
November 15-17, 1971

I. INTRODUCTION

A Seminar on Evaluation, Compilation, and Presentation of Physical Property Data and Data Center Activities was held under the auspices of the Science and Technology Agency of Japan and the National Science Foundation, as an activity of the United States-Japan Scientific Cooperation Program in its Category 3 - Scientific Communication. Its stated purpose was to bring together scientists from the two countries who are concerned with evaluation and dissemination of physical property data, in order that they might exchange information on current activities and explore possibilities for mutually beneficial cooperation. The seminar lasted three days and included 23 formal lectures plus extensive discussion, as well as numerous informal meetings.

The full list of participants is given below. The U.S. Delegation was made up principally of individuals who have been associated in some way with the National Standard Reference Data System. The Japanese Delegation included several who have been involved with data evaluation groups in the U.S. or with international groups such as CODATA. There was a strong representation of chemists among the Japanese, as well as a number of mechanical engineers. Physics, especially the nuclear area, seemed under-represented.

II. LIST OF PARTICIPANTS

U.S. DELEGATION - Dr. Allen V. Astin, Coordinator

1. Dr. Allen V. Astin
   Director Emeritus
   National Bureau of Standards

2. Dr. Edward L. Brady
   Associate Director for Information Programs
   National Bureau of Standards

3. Dr. D. Garvin
   Coordinator for Data Evaluation Programs
   Physical Chemistry Division
   Institute for Materials Research
   National Bureau of Standards

4. Dr. L. J. Kieffer
   Astrophysics Division
   Boulder Laboratories
   National Bureau of Standards

5. Dr. H. William Koch
   Director
   American Institute of Physics

6. Dr. D. R. Lide, Jr.
   Chief, Office of Standard Reference Data
   National Bureau of Standards

7. Dr. Y. S. Touloukian
   Director
   Thermophysical Properties Research Center
   Distinguished Atkins Professor of Engineering
   School of Mechanical Engineering

8. Dr. D. D. Wagman
   Physical Chemistry Division
   Institute for Materials Research
   National Bureau of Standards

9. Prof. E. F. Westrum, Jr.
   Department of Chemistry
   University of Michigan

PARTICIPANTS FROM OTHER COUNTRIES

1. Dr. R. N. Jones
   National Research Council
   CANADA

JAPANESE DELEGATION - Dr. Masao Kotani, Coordinator

1. Prof. Hideaki Chihara
   Department of Chemistry
   Osaka University

2. Prof. Soshin Chikazumi
   Institute for Solid State Physics
   University of Tokyo

3. Prof. Shizuo Fujiwara
   Department of Chemistry
   University of Tokyo

4. Prof. Mitsuho Hirata
   Department of Chemical Engineering
   Tokyo Metropolitan University

5. Dr. Kenzo Hirayama
   Director
   Technical Information Service
   Fuji Photo Film Co., Research Laboratory

6. Prof. Sukeaki Hosoya
   Institute for Solid State Physics
   University of Tokyo

7. Dr. Tomoyoshi Kawada
   Director
   National Research Institute for Metals

8. Prof. Yuichi Kawada
   Department of Mechanical Engineering
   Tokyo Metropolitan University

9. Prof. Koreo Kinoshita
   Department of Physics
   Gakushuin University

10. Prof. Shotaro Kodama
    Department of Mechanical Engineering
    Tokyo Metropolitan University

11. Dr. Masao Kotani
President
Science University of Tokyo

12. Prof. Kozo Kuchitsu
Department of Chemistry
University of Tokyo

13. Prof. Tadashi Makita
Department of Chemical Engineering
Kobe University

14. Dr. Yo-ichiro Mashiko
Director
National Chemical Research Institute for Industry

15. Prof. Akira Nagashima
Department of Mechanical Engineering
Keio University

16. Prof. Jiro Osugi
Department of Chemistry
Kyoto University

17. Prof. Takehiko Shimanouchi
Department of Chemistry
University of Tokyo

18. Prof. Yoshio Takeuchi
Mineralogical Institute
University of Tokyo

19. Prof. Ichimatsu Tanishita
Department of Mechanical Engineering
Keio University

20. Prof. Mitsuo Tasumi
Department of Biophysics and Biochemistry
University of Tokyo

21. Dr. Toshikazu Tsuchiya
Head, Second Division
National Chemical Research Institute for Industry

22. Prof. Koichi Watanabe
Department of Mechanical Engineering
Keio University

23. Dr. Susumu Yoshida
Head, Materials Testing Division
National Research Institute for Metals

24. Prof. Yasuhide Yukawa
Institute of Scientific and Industrial Research
Osaka University

OBSERVERS AND STAFF

1. Dr. Arthur F. Findeis
Staff Associate, NSF/Tokyo Office

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Scientific Attache
American Embassy, Tokyo

3. Mr. James Hoyt
Special Assistant to the Ambassador for
Cultural Affairs
American Embassy, Tokyo

4. Mr. Masanobu Miyahara
Scientific Affairs Advisor
NSF/Tokyo Office

5. Dr. Toshiharu Tako
Head of Second Division
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8. Mr. Masaji Sawabe
Principal Research Officer Laboratory of Metrology

9. Miss Teruko Inamatsu
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National Research Laboratory of Metrology

10. Prof. Tatsuo Miyazawa
Institute for Protein Research
Osaka University

11. Prof. Takashi Shimozawa
Department of Chemistry
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CHAIRMAN OF THE EXECUTIVE COMMITTEE OF RIAC

1. Prof. Masamichi Tsuboi
Faculty of Pharmaceutical Sciences
University of Tokyo

2. Prof. Ichiro Nakagawa
Department of Chemistry
University of Tokyo

MEMBER OF EXECUTIVE COMMITTEE OF IRDC

1. Dr. Shigeru Yamauchi
Department of Industrial Chemistry
University of Tokyo

2. Dr. Tomoko Nakahara
Department of Chemical Engineering
Tokyo Metropolitan University

3. Miss Derothy U. Mizoguchi
Chief
Cancer Chemotherapy Information Center

SCIENCE AND TECHNOLOGY AGENCY

1. Mr. Yoshiro Narabayashi
Director General
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   Promition Bureau

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   Head of Administration Division
   Promotion Bureau

9. Mr. Takashi Hironaka
   Chief of Information Section
   Promotion Bureau

III. PROGRAM

MONDAY - November 15, 1971

Morning: Session 1 (10:00 a.m. - 12:00 noon)

1. Welcome Address by Representative of Japanese Implementing Agency

   Mr. Yoshiro Narabayashi
   Director General
   Planning Bureau
   Science and Technology Agency

2. Addresses by Representative of Participants from Japan and U.S.

   Dr. M. Kotani
   President
   Science University of Tokyo

   Dr. A. V. Astin
   Director Emeritus
   National Bureau of Standards

3. Adoption of Agenda

4. Presentation and Discussion of Papers
   (1) Data Handling in Primary Publications in Japan

Prof. H. Chihara
Department of Chemistry
Osaka University

Executive Secretary
Japanese CA Abstractors Association

(2) Presentation of Concepts and Numerical Data in Physics

Dr. H. William Koch
Director
American Institute of Physics

Afternoon: Session 2 (2:00 - 5:00 p.m.)

(3) Rationale and Development of the U.S. National Standard Reference Data System

Dr. Edward L. Brady
Associate Director for Information Programs
National Bureau of Standards

(4) Present Status of the U.S. Standard Reference Data Program

Dr. D. R. Lide, Jr.
Chief, Office of Standard Reference Data
National Bureau of Standards

(5) Data Center Activity on Molecular Vibrations

Prof. T. Shimanouchi
Department of Chemistry
University of Tokyo

(6) Collection and Evaluation of Molecular Vibrational Frequencies

Prof. M. Tasumi
Department of Biophysics and Biochemistry
University of Tokyo

(7) Functions of High Pressure Data Center

Prof. J. Osugi
Department of Chemistry
Kyoto University

TUESDAY - November 16, 1971

Morning: Session 3 (9:30 a.m. - 12:00 noon)

(8) The Thermophysical Properties Research Center
Its Aims and Activities

Dr. Y. S. Touloukian
Director
Thermophysical Properties Research Center
Distinguished Atkins Professor of Engineering
School of Mechanical Engineering

(9) Evaluation of Experimental Data for Thermodynamic
Properties of Fluorocarbon Refrigerants

Prof. I. Tanishita
Prof. K. Watanabe
Division of Mechanical Engineering
Keio University

(10) Critical Evaluation of Data in Chemical Thermodynamics

Dr. D. D. Wagman
Physical Chemistry Division
Institute for Material Research
National Bureau of Standards

(11) Collection of Data on Fatigue Strength of Metals
and the Need of Their Statistical Treatment

Prof. Y. Kawada
Department of Mechanical Engineering
Tokyo Metropolitan University

Afternoon: Session 4 (2:00 - 5:00 p.m.)

(12) Collection and Evaluation of Electron Diffraction Data

Prof. K. Kuchitsu
Department of Chemistry
University of Tokyo

(13) Measurement Techniques and the Evaluation of Property Data

Dr. L. J. Kieffer
Astrophysics Division
Boulder Laboratories
National Bureau of Standards

(14) Evaluation of X-ray Diffraction Data

Prof. S. Hosoya
Institute for Solid State Physics
University of Tokyo

(15) Criteria for Reporting Property Measurements in the Literature

Prof. E. F. Westrum, Jr.
Department of Chemistry
University of Michigan

(16) Present Status of Activities for Collection and Distribution of Mass Spectral Data in Japan

Dr. T. Tsuchiya
Head
Second Division
National Chemical Research Institute for Industry

WEDNESDAY - November 17, 1971

Morning: Session 5 (9:30 a.m. - 12:00 noon)

(17) Computer Storage and Search of Spectral Data

Dr. R. N. Jones
National Research Council
Canada

(18) Long-Term Creep Data on Domestic Materials Obtained at National Research Institute for Metals

Dr. T. Kawada
Director
National Research Institute for Metals

Dr. S. Yoshida
Head
Materials Testing Division
National Research Institute for Metals

(19) Complete Clear Text Representation of Scientific Documents in Machine-Readable Form

Dr. D. Garvin
Coordinator for Data Evaluation Programs
Physical Chemistry Division
Institute for Materials Research
National Bureau of Standards

(20) Compilation and Computer Estimation of Physical Property Values for Chemical Engineers

Prof. M. Hirata
Department of Chemical Engineering
Tokyo Metropolitan University

Afternoon: Session 6 (2:00 - 5:00 p.m.)

(21) A Plan of Data Depository Center for Organic Chemistry

Prof. Y. Yukawa
Institute of Scientific and Industrial Research
Osaka University

(22) Necessity of Establishing Data (Service) Center in Japan

Dr. Y. Mashiko
Director
National Chemical Research Institute for Industry

(23) Opportunities for U.S. - Japan Cooperative Projects

Dr. D. R. Lide, Jr.
Chief, Office of Standard Reference Data
National Bureau of Standards

IV. SUMMARY OF U.S. PAPERS

The papers presented by the U.S. Delegation fell into three categories: data evaluation under the NSRDS program, reporting of data in the primary literature, and the use of computers in data processing. The background of the National Standard Reference Data System and the philosophy of its operation were described by E. L. Brady, and current activity under the program was summarized by D. R. Lide. Particular emphasis was given to problems of dissemination of reference data. D. D. Wagman discussed the procedures followed by the Chemical Thermodynamics Data Center in evaluating

a large ensemble of highly interrelated data. There was also a discussion of the activity of CODATA in establishing standard values of thermodynamic properties of key substances. A different aspect of the evaluation problem was described by L. J. Kieffer, who stressed the difficulty in assessing the contribution of various sources of systematic error. The importance of having a thoroughly understood and completely documented theory of the experiment was brought out in this talk. Y. S. Touloukian discussed the problems of operating a large information analysis center in which information retrieval, data evaluation, and experimental and theoretical research are highly integrated.

Some aspects of the presentation of results of experimental measurements were discussed by two speakers. H. W. Koch described plans of the American Institute of Physics to develop more effective means of distributing primary and secondary information to the physics community. E. F. Westrum stressed the need for more complete reporting of the results of experimental measurements in the primary literature. He described the work of thermodynamicists in drawing up a "Guide to the Publication of Thermodynamic Data" which gives detailed instructions on the way in which data should be reported and the auxiliary information which should be supplied.

The role of modern computers in data handling was discussed by two speakers. R. N. Jones (who was present as a third-country representative from Canada) discussed the computer storage and retrieval of spectral data. He stressed the importance of setting uniform formats for reporting spectral data of all types and for insuring the technical quality of the data before

it went into a computer storage bank. D. Garvin described the General Purpose Scientific Document Image Code, a system for storing scientific data and text in a manner which permits great flexibility of output.

V. SUMMARY OF JAPANESE PAPERS

Although most of the Japanese papers dealt with specific technical areas, three speakers covered more general problems. H. Chihara discussed the presentation of data in the primary literature, stressing the need for journal editors to exert better quality control over the papers which they publish. He also described efforts in Japan to make original experimental data available to evaluators when it is too bulky to publish in regular journals. There was also a discussion of Japanese contributions to the preparation of abstracts for Chemical Abstracts.

A proposal for establishing a large data distribution center in Japan was presented by Y. Mashiko. The center would collect and index data compilations from all parts of the world and maintain contact with data evaluation centers. Inquiries for data and other information would be answered from the resources of the center. Y. Yukawa described plans for an organic chemistry data depository center. This center would collect data of various types -- spectral, thermodynamic, physical properties, etc. -- classified by compound and make it available to inquirers. The aim appeared to be to establish a comprehensive, but not necessarily critical depository, although cooperation with data evaluation centers was mentioned. Neither of these proposals seemed to have reached the stage of concrete planning,

especially as regards financial considerations.

Data evaluation activities in several specific technical areas were described by the other Japanese participants. Vibrational spectroscopy was covered by T. Shimanouchi and M. Tasumi. They discussed the Japanese collection of infrared spectral data (IRDC), bibliographic activities on infrared and Raman spectroscopy, collections of force constants, and the preparation of tables of molecular vibrational frequencies. The latter project is carried out as part of the NSRDS program. T. Tsuchiya discussed mass spectral data and outlined the way in which Japanese activities fitted into the international program on mass spectral data collection. A Japanese group has published three annual indices to the literature of organic mass-spectra, but the project has encountered financial difficulties. There were two talks in the area of molecular structure. K. Kuchitsu discussed structural data obtained by gas-phase electron diffraction; he described existing bibliographic activities and pending evaluation projects of an international nature. In view of the great research activity in this field in Japan, a strong input to compilation and evaluation is hoped for. Evaluation of X-ray diffraction data on solids was discussed by S. Hosoya. Here Japanese groups have been cooperating with other national and international groups in standardizing measurements and developing data files.

J. Osugi described the High Pressure Data Center of Japan, which works closely with its U.S. equivalent at Brigham Young University. These two groups exchange information on high pressure phenomena on a regular basis.

Evaluation of equation of state data on fluorocarbon refrigerants was described in some detail by I. Tanishita, K. Watanabe, H. Kondo, and K. Oguchi. Japanese efforts on properties of fluids of interest to chemical engineers were outlined by M. Hirata. These include publication of an annual summary of physical properties retrieved from the primary literature and development of a computer program for estimation and retrieval of property data.

Finally, two papers were devoted to mechanical property data. Y. Kawada discussed the collection of data on the fatigue strength of metals, stressing particularly the need for a statistical approach because of the variability found over a range of samples. A program for collecting long-term creep data on structural materials was described by T. Kawada and S. Yoshida. In its present form, this involves testing of samples in a central laboratory under standardized procedures. Data sheets will be published annually beginning in 1972.

VI. SUMMARY AND PROGNOSIS FOR FUTURE COOPERATION

It is evident from the above outline of the symposium that there is considerable data compilation activity in Japan, but that the coverage of technical areas is rather spotty. In the absence of any central coordinating body, data centers and other evaluation activities have grown up on the initiative of individual Japanese scientists, often with influence from foreign groups. The difficulty in obtaining stable funding, or even clear directives, from government or industry is apparent. Several

projects appeared to suffer from inadequate funding, and some publication series had ceased after the first two or three years. On the other hand, there seemed to be a strong market for data and other technical information in Japan; the circulation figures for some of the publications mentioned at the symposium were quite impressive.

All of the Japanese participants seemed to feel, not surprisingly, that the Japanese Government should provide more funds for data compilation and evaluation. However, there were a variety of views on the way these funds should be spent. Some participants hoped for more support for individual data evaluation projects, particularly in the universities. Interest was expressed in setting up data centers, on the NSRDS model, in a number of technical areas. Other speakers emphasized the need for funds for a central service organization, covering a broad scope, which would respond to requests for data.

One point which emerged from the symposium was that a significant amount of U.S.-Japanese cooperation already exists in the data field. Examples of activities in which Japanese and U.S. groups cooperate on a regular basis include:

1. Molecular vibrational frequencies - T. Shimanouchi, University of Tokyo compiles data for publication in the NSRDS series.
2. Thermochemistry - Y. Takahashi, University of Tokyo, contributes to the Annual Bulletin of Thermodynamics and Thermochemistry, edited by E. F. Westrum, University of Michigan.
3. Viscosity and specific heat - T. Makita, Kobe University, evaluates data for Thermophysical Properties Research Center, Purdue University.

4. High pressure data - J. Osugi, Kyoto University, exchanges information with High Pressure Data Center, Brigham Young University.

5. Molecular structure - bibliography on gas phase molecular structure is being prepared as multi-national effort to which K. Kuchitsu, University of Tokyo, and W. H. Kirchhoff, National Bureau of Standards are making major input.

These and other examples of working cooperation have developed spontaneously as a result of a confluence of interests on the part of individual scientists in the two countries. Some of the arrangements have been operating very effectively for a number of years.

If a formal data program is established by the Japanese Government in the future, there will undoubtably be increased opportunities for collaboration. From the viewpoint of cooperation at the planning level, it would be desirable to have a central focal point in Japan similar to the NBS Office of Standard Reference Data in the U.S. We could establish procedures for routine exchange of information, exchange of proposals for review, and take other steps to insure against unnecessary duplication of effort. An interaction of this type between the Office of Standard Reference Data and the Office of Scientific and Technical Information (OSTI) in the United Kingdom has proved very effective. A similar arrangement between the U.S. and Japan should be helpful to both sides.

In addition to the areas listed above where substantive collaboration between U.S. and Japanese groups already exists, several other possibilities for joint projects presented themselves during the symposium. Among the more promising areas are:

1. Interatomic distances - There is strong interest and considerable competence in Japan in the determination of interatomic distances by diffraction and spectroscopic methods. An international effort to prepare tables of evaluated structural data has been proposed. It is reasonable to expect the U.S. and Japan to play a major part.
2. Thermodynamic properties of fluids - Possibilities for collaboration under various international programs.
3. Mechanical properties - Activities planned in U.S. might be coordinated with existing Japanese program.
4. Magnetic properties of solids - There is interest in Japan in starting compilation in this area, where there is now little activity in the U.S.
5. Nuclear magnetic resonance - Interest in compilation projects exists in both countries. This is a very large area, which could usefully be partitioned.
6. Photochemistry - This is an active research field in Japan, and data program might be developed which would mesh with chemical kinetics program in the U.S.

Other areas such as mass spectroscopy, gas chromatography, and infrared spectroscopy also offer possibilities for joint projects. On a different level, the present arrangement for providing abstracts from the Japanese literature to Chemical Abstracts might be extended to other disciplines. Finally, it seems desirable to consult on computer formats for handling

data. Adoption of common formats at an early stage will simplify data exchange between centers in the two countries.

Extended abstracts of the papers presented at the Symposium are attached.

REPORT SUBMITTED BY: Dr. David R. Lide, Jr., Chief
Office of Standard Reference Data
National Bureau of Standards

March 27, 1972